Simulation of Type-II Ge/Si Quantum Dot Solar Cells

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INTRODUCTION

Silicon solar cells have faced their limitation of conversion efficiency for many years. Quantum dot solar cell brings us a great interest to break this frustrating limitation. Combining neutral beam etching with bio-template, advanced nano-process technique was utilized to fabricate superlattices; in particular, for Si nanodisk array [1]. In this study, a 3D finite element method (FEM) is advanced for type-II Ge/Si quantum dot solar cells, which is integrated into the detailed balance transport equation to calculate the conservation efficiency of intermediate band solar cell (IBSC) [2-4].

THE COMPUTATIONAL MODEL

The electronic structure is solved on the basis of envelope-function approximation [3-4]:

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + V\right)\psi = E\psi. \quad (1)$$

In the IBSC, the electron conduction current is described as the continuty functions:

$$\frac{dn}{dt} = (G_{VC} - R_{VC}) + (G_{IC} - R_{IC}) + \frac{1}{q}\frac{dJ_n}{dx}. \quad (2)$$

Photovoltage V equals to quasi fermi level splitting between the conduction and valence bands.

$$V = \mu_{VC} = Ef_C - Ef_V. \quad (3)$$

The detailed balance process determines the carrier's chemical potential:

$$G_{VI}(x) - R_{VI}(x) = G_{IC}(x) - R_{IC}(x). \quad (4)$$

RESULTS AND DISCUSSION

As shown in Fig. 1(a), Ge/Si is a typical type-II quantum structure under stress-free conditions. The hole was strongly localized in the Ge QD with a 0.095-eV ground-confined level; however, electrons freely moved in the Si matrix. In a realistic structure, the large lattice mismatch generally induces compressive stress, as shown in Fig. 1(b), which slightly confines the electrons. This additional confinement enhances the optical transition matrix significantly. The 3D FEM simulation enables us to calculate stress distribution. Figure 2 shows the miniband formation in a Ge/Si QD superlattice. Several clear minibands are evident. The miniband induced by the heavy holes ground state are substantially separated from the continuous valence band and other minibands, which have sub-bandgaps several tens of times larger than the thermal energy. With the suggested device structure in Fig. 3, we calculated the I-V curves, as shown in Fig. 4. Under one-sun, the Si QD only improved the efficiency very little, as shown in Fig. 5; however, under the concentration application, the most attractive commercial applications, its conversion efficiency drastically increase to more than 42% under 200X concentration. As shown in Fig. 6, for one-sun applications, H-passivation Si or regrowthing amorphous Si has a great potential to achieve 45%.

CONCLUSION

Ge/Si QD superlattice is especially for concentration application; and with H-passivation Si or regrowth to fabricate amorphous Si matrix, it has a potential to achieve 45% under 1-sun.

ACKNOWLEDGEMENT

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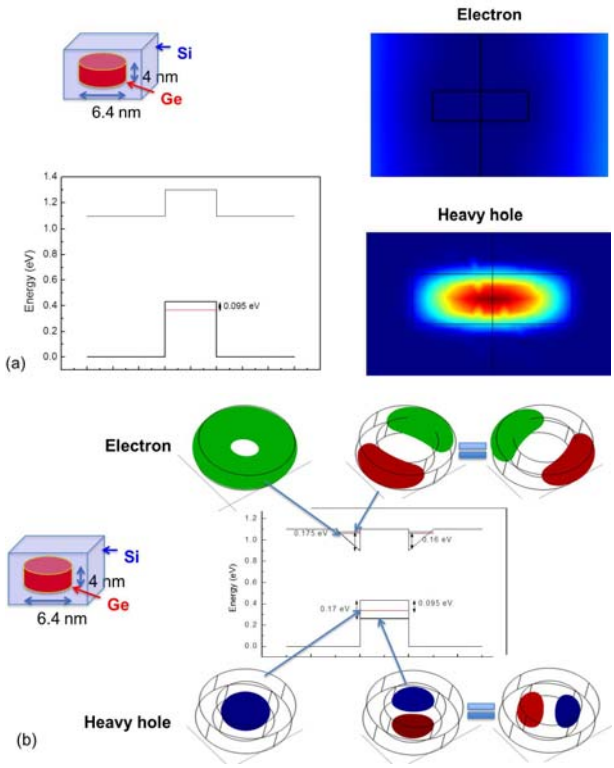

Fig. 1. The quantum level and wavefunction in single Ge/Si QD (a) without stress and (b) with stress.

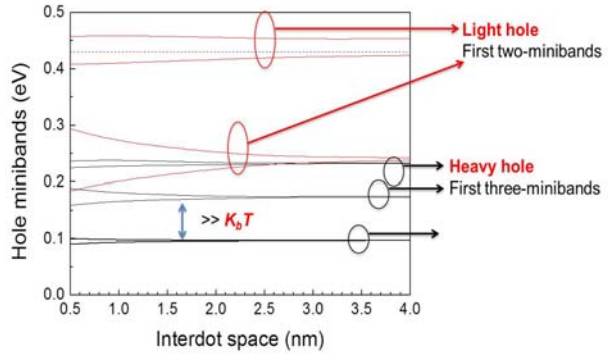

Fig. 2. The miniband formations in the Ge/Si QD superlattice.

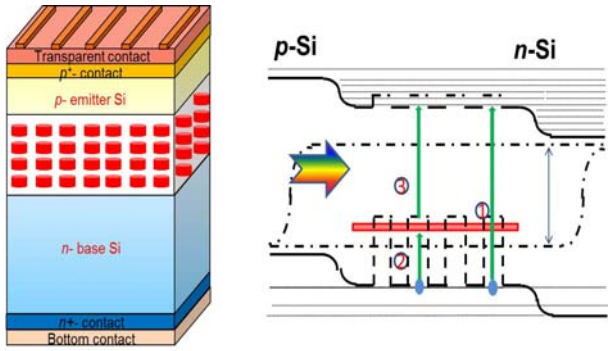

Fig. 3. The explored Ge/Si IBSC's device structure for solar cell applications and the corresponding band profile.

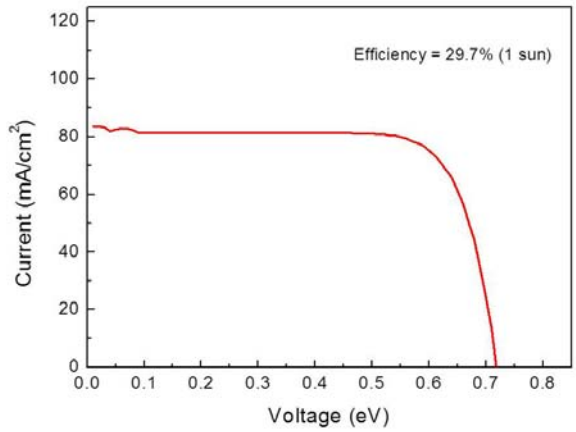

Fig. 4. The simulated I-V profile of the Ge/Si IBSC (one-sun, 5800 K blackbody).

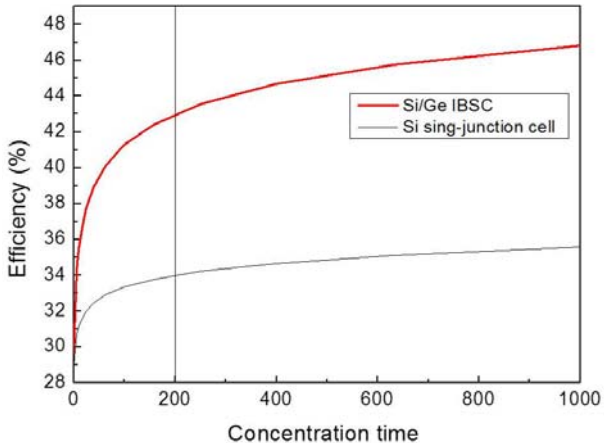

Fig. 5. The plot of conversion efficiency as a function of concentration time. The proposed structure possesses the improved conversion efficiency compared with the conventional one.

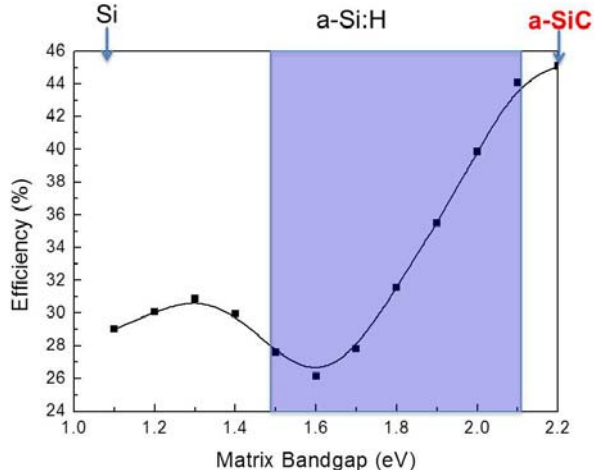

Fig. 6. The conversion efficiency under one-sun as a function of matrix bandgap. With H-passivation treatment, amorphous Si bandgap would gradually increase to 2.1 eV, and thus, the conversion efficiency has a potential to approach 45%.